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Quantum tunneling in thermal medium

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ABSTRACT

Time evolution of tunneling phenomena in medium is studied using a standard model of environment interaction. A semiclassical formula valid at low, but finite temperatures is derived in the form of integral transform for the reduced Wigner function, and the tunneling probability in thermal medium is calculated for a general tunneling potential of one dimensional system. Effect of dissipation, its time evolution in particular, depends on the behavior of the potential far beyond the barrier.

Tunneling phenomena are genuinely a quantum effect. When they occur in some surrounding medium, the important question arises as to whether the tunneling rate is enhanced or suppressed by the environment effect. There are already many works on this subject [1], and most past works deal with a system in equilibrium as a whole. The Euclidean technique such as the bounce solution [2] is often used in this context [3], [4]. Our approach here is different, and we attempt to clarify dynamics of time evolution starting from an arbitrary initial state of the tunneling system, which can be either a pure or a mixed state. Moreover we find it more illuminating to use a real-time formalism instead of the Euclidean method much employed in the literature [5].

Although one can think of many applications of our general framework here, application to cosmology is our prime target [6]. The cosmological environment is in many aspects the simplest since the environment is almost spatially homogeneous and for many purposes its state can be characterized by a single temperature parameter. Furthermore cosmic evolution gives rise to decrease of the temperature, dropping some degree of freedom out of equilibrium with the rest. This gives a natural setting for separation of a subsystem from the environment, which is at the heart of our approach.

The standard model [7],[3] of environment and its interaction with a one dimensional system which we describe by a potential $V(q)$ introduces an infinitely many, continuous harmonic oscillators of environment and a bilinear interaction, $q\int d\omega\, c(\omega)Q(\omega)$. Here $Q(\omega)$ is the environment oscillator coordinate of frequency ω and $c(\omega)$ gives a coupling strength of the system-environment interaction. Although the form of interaction seems rather limited, it is generally believed that details of the environment interaction with the system should not be important and this form should suffice. With the total system specified, dynamics is given by the quantum equation of motion,

$$\frac{d^2q}{dt^2}+\frac{dV}{dq}=-\int_{\omega_c}^{\infty} d\omega\, c(\omega)Q(\omega)\,,\qquad \frac{d^2Q(\omega)}{dt^2}+\omega^2\,Q(\omega)=-\,c(\omega)q\,. \tag{1}$$

Quantum Langevin equation is derived [8] by eliminating the environment variable $Q(\omega\,,t)$;

$$\frac{d^2q}{dt^2}+\frac{dV}{dq}+2\int_0^t ds\,\alpha_I(t-s)q(s)=F_Q(t)\,, \tag{2}$$

where $F_Q(t)$ has an explicit, linear dependence on the initial values, $Q_i(\omega)\,, P_i(\omega)=\dot{Q}_i(\omega)$. In a thermal bath of environment temperature $T=1/\beta$ the random force

from the environment is characterized by the correlation function,

$$\langle \{F_Q(\tau)\,,F_Q(s)\}_+\rangle_{\rm env} = \int_{\omega_c}^{\infty} d\omega\, r(\omega)\cos\omega(\tau-s)\,\coth(\frac{\beta\omega}{2})\,, \tag{3}$$

with $r(\omega)=c^2(\omega)/(2\omega)$. The kernel function α_I in eq.(2) is related to the real-time thermal Green's function and is given by $\alpha_I(t) = -\int_{\omega_c}^{\infty} d\omega\, r(\omega)\sin(\omega t)$.

An often used simplification is the local, Ohmic approximation taking $r(\omega) = \eta\omega/\pi$ with $\omega_c = 0$, which amounts to $\alpha_I(\tau) = \delta\omega^2\delta(\tau) + \eta\,\delta'(\tau)$. This gives $\delta\omega^2\, q + \eta\dot{q}$ in the Langevin equation (2). The parameter $\delta\omega^2$ is interpreted as a potential renormalization effect or the mass renormalization in the field theory analogy, while η is the Ohmic friction coefficient. This approximation breaks down at early times [9], but it is useful in many other cases.

Our discussion starts from the master equation for this system, which is written for convenience in terms of the Wigner function $f_W(q\,,p\,,Q(\omega)\,,P(\omega))$, a Fourier transformation of the density matrix $\rho(q\,,q'\,,Q(\omega)\,,Q'(\omega))$ with respect to the relative coordinate, $q-q'\,,\ Q(\omega)-Q'(\omega)$,

$$\begin{aligned}\frac{\partial f_W}{\partial t} &= -p\frac{\partial f_W}{\partial q} - \int d\omega\,\left(P(\omega)\frac{\partial f_W}{\partial Q(\omega)} + c(\omega)\,(q\frac{\partial}{\partial P(\omega)} + Q(\omega)\frac{\partial}{\partial p})\,f_W\right)\\ &+ \frac{1}{i\hbar}\left\{ V\left(q+\frac{i\hbar}{2}\frac{\partial}{\partial p}\right) - V\left(q-\frac{i\hbar}{2}\frac{\partial}{\partial p}\right)\right\} f_W\,. \end{aligned}\tag{4}$$

The crucial observation for subsequent development is how the Planck constant $\hbar$ enters in the master equation (4). In one dimensional quantum mechanics the semiclassical approximation is excellent when the potential barrier is large, and we assume that this is also true in the presence of the system-environment interaction. In the semiclassical $\hbar\to 0$ limit we have

$$\frac{1}{i\hbar}\left\{ V\left(q+\frac{i\hbar}{2}\frac{\partial}{\partial p}\right) - V\left(q-\frac{i\hbar}{2}\frac{\partial}{\partial p}\right)\right\} f_W \;\to\; \frac{dV}{dq}\,\frac{\partial f_W}{\partial p}\,. \tag{5}$$

The resulting equation, being identical to the classical Liouville equation, has an obvious solution;

$$\begin{aligned} f_W(q\,,p\,,Q\,,P) = \int dq_i dp_i \int dQ_i dP_i\, f_W^{(i)}(q_i\,,p_i\,,Q_i\,,P_i)\\ \cdot\delta\,(q-q_{\rm cl})\;\delta\,(p-p_{\rm cl})\;\delta\,(Q-Q_{\rm cl})\;\delta\,(P-P_{\rm cl})\;, \end{aligned}\tag{6}$$

where $q_{\rm cl}(q_i\,,p_i\,,Q_i\,,P_i\,;t)$ etc. are the solution of (1), taken as the classical equation.

We consider the circumstance under which the tunneling system is initially in a state uncorrelated to the rest of environment. Thus we take an uncorrelated initial

state of the form $\rho^{(i)} = \rho_q^{(i)} \otimes \rho_Q^{(i)}$, to get the reduced Wigner function after the trivial $Q(\omega)\,, P(\omega)$ integration,

$$f_W^{(R)}(q\,,p\,;t) = \int dq_i dp_i\, f_{W\,,q}^{(i)}(q_i\,,p_i)\, K(q\,,p\,,q_i\,,p_i\,;t)\,,$$
$$K(q\,,p\,,q_i\,,p_i\,;t) = \int dQ_i dP_i\, f_{W\,,Q}^{(i)}(Q_i\,,P_i)\,\delta\,(q-q_{\rm cl})\;\delta\,(p-p_{\rm cl})\;. \qquad (7)$$

The problem of great interest is how further one can simplify the kernel function K here.

In many situations one is interested in the tunneling probability when the environment temperature is low enough. At low temperatures of $T \ll$ a typical frequency or curvature scale ω_s of the potential V, one has $\omega_s \sqrt{\overline{Q_i^2(\omega)}}\,, \sqrt{\overline{P_i^2(\omega)}} = O[\sqrt{T}] \ll \sqrt{\omega_s}$. Expansion in terms of $Q_i(\omega)\,, P_i(\omega)$ is then justified. Thus, we use

$$\delta\,(\,q-q_{\rm cl}\,) = \int \frac{d\lambda_q}{2\pi}\,\exp\,[\,i\,\lambda_q\;(\,q-q_{\rm cl}\,)\,]$$
$$\approx \int \frac{d\lambda_q}{2\pi}\,\exp\left[\,i\,\lambda_q\,\left(\,q-q_{\rm cl}^{(0)} - \int d\omega\,\left\{\,Q_i(\omega) q_{\rm cl}^{(Q)}(\omega) + P_i(\omega)\,q_{\rm cl}^{(P)}(\omega)\,\right\}\right)\right]\,, \qquad (8)$$

valid to the first order of $Q_i(\omega)\,, P_i(\omega)$. A similar expansion for $\delta\,(\,p-p_{\rm cl}\,)$ using $p_{\rm cl}^{(0)}\,, p_{\rm cl}^{(Q)}(\omega)\,, p_{\rm cl}^{(P)}(\omega)\,,$ also holds.

Gaussian integral for the variables $Q_i(\omega)\,, P_i(\omega)\,, \lambda_q\,, \lambda_p$ can be done explicitly with eq.(8), when one takes the thermal density matrix for the initial environment, $\rho_Q^{(i)}$. The result of this Gaussian integral leads to an integral transform of the Wigner function, $f_W^{(i)} \to f_W^{(R)}$, using the kernel function of

$$K(q\,,p\,,q_i\,,p_i\,;t) = \frac{\sqrt{\det\,\mathcal{J}}}{2\pi}\,\exp\left[\,-\frac{1}{2}(q-q_{\rm cl}^{(0)}\,,\,p-p_{\rm cl}^{(0)})\,\mathcal{J}\,\begin{pmatrix} q-q_{\rm cl}^{(0)} \\ p-p_{\rm cl}^{(0)}\end{pmatrix}\right]\,, \qquad (9)$$

where the matrix elements of $\mathcal{J}^{-1} = I_{ij}$ are given by

$$I_{11} = \frac{1}{2}\int_{\omega_c}^{\infty} d\omega\,\coth\frac{\beta\omega}{2}\,\frac{1}{\omega}\,|z(\omega\,,t)|^2\,, \qquad (10)$$
$$I_{22} = \frac{1}{2}\int_{\omega_c}^{\infty} d\omega\,\coth\frac{\beta\omega}{2}\,\frac{1}{\omega}\,|\dot{z}(\omega\,,t)|^2\,, \qquad (11)$$
$$I_{12} = \frac{1}{2}\int_{\omega_c}^{\infty} d\omega\,\coth\frac{\beta\omega}{2}\,\frac{1}{\omega}\,\Re\,(z(\omega\,,t)\dot{z}^*(\omega\,,t))\;, \qquad (12)$$

where $z(\omega\,,t) = q_{\rm cl}^{(Q)}(\omega\,,t) + i\,\omega\,q_{\rm cl}^{(P)}(\omega\,,t)\,,$ and $\dot{z}(\omega\,,t) = p_{\rm cl}^{(Q)}(\omega\,,t) + i\omega\,p_{\rm cl}^{(P)}(\omega\,,t)\,.$

Quantities that appear here ought to be determined by solving differential equations with a given initial condition; the homogeneous Langevin equation and its

linearized equation of the form

$$\frac{d^2 q_{\rm cl}^{(0)}}{dt^2} + \left(\frac{dV}{dx}\right)_{q_{\rm cl}^{(0)}} + 2\int_0^t ds\, \alpha_I(t-s) q_{\rm cl}^{(0)}(s) = 0\,, \tag{13}$$

$$\frac{d^2 z(\omega\,,t)}{dt^2} + \left(\frac{d^2 V}{dx^2}\right)_{q_{\rm cl}^{(0)}} z(\omega\,,t) + 2\int_0^t ds\, \alpha_I(t-s) z(\omega\,,s) = -\,c(\omega) e^{i\omega t}\,. \tag{14}$$

The same linear equation as for $z(\omega\,,t)$ holds for $\dot{z}(\omega\,,t)$. The initial condition is $q_{\rm cl}^{(0)}(t=0) = q_i\,, \quad p_{\rm cl}^{(0)}(t=0) = p_i\,, \quad z(\omega\,,t=0) = 0\,, \quad \dot{z}(\omega\,,t=0) = 0\,.$ Once the reduced Wigner function is known, one can compute any physical quantity by a phase space integration.

The physical picture underlying the formula for integral transform should be evident; the probability at a phase space point $(q\,,p)$ is dominated by the semiclassical trajectory (environment effect of dissipation being included for its determination) reaching $(q\,,p)$ from an initial point $(q_i\,,p_i)$ whose contribution is weighed by the quantum mechanical probability $f_W^{(i)}$ initially given. The broadning of the trajectory due to the environment interaction is given by the width factor $\sqrt{I_{ij}}$.

To proceed further, we distinguish two cases of the potential type, depending on the value of $V(\infty)$ relative to the local minimum value V_m in the potential well. The kind of potential we have in mind is depicted in Fig.1. When $V(\infty) < V_m$ (Fig.1a), the classical motion is usually monotonic ending at $x = \infty$, while for $V(\infty) > V_m$ (Fig.1b) the motion is a damped oscillation towards x_0 at the true minimum, unless the friction is large. If the friction is larger than a critical value of $\approx 2\omega_0$ with ω_0 given by the curvature of the potential at the global minimum, there occurs the overdamping such that $q_{\rm cl}^{(0)} \to x_0$ monotonically. A typical interesting case for $V(\infty) > V_m$ is the asymmetric double well as may occur in the first order electroweak phase transition [6].

In the rest of this paper, we consider a few problems to illustrate consequences of our general formula of the integral transform. One problem is the outgoing flux to the overbarrier region of the type of potential of Fig.1a, assuming an initial energy eigenstate under the whole potential V. The other problem is the tunneling probability for the type of potential of Fig.1b. We take here an initial thermal state of the same temperature as the environment, given by the density matrix $\propto \sum_n e^{-\beta E_n} |n\rangle\langle n|$ with $|n\rangle$ the exact energy eigenstate under V. This choice is made in order to mimic the cosmological first order phase transition in which the local minimum in the left was the true minimum above a critical temperature. We insist on the energy eigenstate because it is the most stable state, being stationary when the environment

interaction is switched off. In this sense the choice of the energy eigenstate and its mixture is useful in many applications.

We first discuss the tunneling probability for the case of $V(\infty) < V_m$. Suppose that we are primarily interested in the tunneling probability from a state localized in the left well into the right region far beyond the barrier. For discussion from further on we assume $\omega_* \ll V_h$, where ω_* is the frequency defined at the potential bottom in the well and V_h the barrier height seen from the bottom. Since higher energy states contribute roughly with the weight factor, $e^{-2H(q_i\,,p_i)/\omega_*}$, where $H(q_i\,,\,p_i)$ is the hamiltonian of the hypothetical oscillator of frequency ω_* without the barrier in the right, the high momentum component above the barrier is suppressed by $e^{-\,2V_h/\omega_*}$. We assume that this factor is much smaller than a typical barrier penetration factor $|T(E)|^2$ in the overbarrier region, usually given by the WKB formula, $\exp[-2\int dx|p(x)|\,]$. In this way we may restrict the phase space region in the integral transform to the region D defined by $|V_0| < \frac{1}{2}\,p_i^2 + \frac{1}{2}\,\omega_0^2\,(q_i - x_0)^2 < V_h + |V_0|\,,$ with V_0 the minimum potential value at x_0.

The flux at x is calculated from an integral of the form, $\sim \int dp\,p\,f_W^{(R)}(x\,,p\,;t)\,,$ giving

$$I(x\,,t) \;=\; \int_D dq_i\,dp_i\,f_W^{(i)}(q_i\,,p_i)\,\frac{1}{\sqrt{2\pi I_{11}}}\,\exp\left[-\frac{(x-q_{\rm cl}^{(0)})^2}{2I_{11}}\right] \cdot\left(\,p_{\rm cl}^{(0)} + \frac{I_{12}}{I_{11}}\,(x-q_{\rm cl}^{(0)})\,\right)\,. \tag{15}$$

The initial Wigner function $f_W^{(i)}(q_i\,,p_i)$ is a Fourier transform of $\psi^*(q_i - \frac{\xi}{2})\psi(q_i + \frac{\xi}{2})$ with respect to ξ, where ψ is the initial wave function. The phase of the wave function plays an important role for the region, $q_i > x_*$ where x_* is a turning point in the overbarrier region, and one may use the stationary phase approximation for the ξ and p_i integration. We find a stationary point at $\xi = 0\,, \quad p_i = I(q_i)\,, \quad I(x) = \frac{-i}{2}\,(\,\psi^*(x)\psi'(x) - \psi'^{\,*}(x)\psi(x)\,)\,/|\psi(x)|^2\,.$ The quantity $I(x)$ is the usual quantum mechanical flux associated with the initial quantum state.

In the region of $x \gg x_*$ there is always a classical trajectory that reaches the point x of the Gaussian peak from an initial q_i in the range $q_i > x_*$, and the entire region within the Gaussian width $\sqrt{I_{11}}$ is fully covered by the integral. The factor outside the Gaussian exponent is well approximated by its peak value in the weak coupling case. Thus, one obtains $I(x\,,t) \approx |\psi(x_c)|^2\,(-\dot{x}_c)\,,$ where one determines $x_c(x\,,t)$ from $q_{\rm cl}^{(0)}(x_c\,,I(x_c)\,,0\,,0\,;t) = x\,.$ Using the WKB wave function for the energy eigenstate at $q_i > x_*,\;\; \psi(q_i) = T(E)\exp\left[i\int_{x_*}^{q_i} p(x)\right]/\sqrt{p(q_i)}\,,\;\; p(x) = \sqrt{2(E-V(x))}\,,$

one has a factorized form of the flux;

$$I(x\,,t) \approx |T(E)|^2\, f(x\,,t\,;E)\,, \quad f = \frac{p_{\rm cl}^{(0)}(x_c\,,t)}{p(x_c)} \left(\frac{dq_{\rm cl}^{(0)}(x_c\,,t)}{dx_c} \right)^{-1} . \tag{16}$$

We note that the potential renormalization effect should be included for $|T(E)|^2$, as emphasized in [3].

This formula for the flux reproduces our previous result for a specific potential of the inverted harmonic oscillator [10], $V(x) = -\frac{1}{2}\,\omega_R^2\, x^2$. In this case the Gaussian integral gives the exact result, relying neither on the low temperature nor on the stationary phase approximation. The present approach actually improves our previous result;

$$f = \frac{\ddot{g}\; x_c + \dot{g} I(x_c)}{\dot{g} I(x_c) + g\omega_B^2 x_c} \to \frac{\ddot{g} + \omega_B \dot{g}}{\omega_B(\dot{g} + \omega_B g)}\,, \tag{17}$$

where $\omega_B \approx \omega_R - \eta/2$ is a diagonalized frequency, and the initial flux $I(x_c) = \sqrt{2(E - V(x_c))}$ in the WKB approximation. The function $g(t)$ is the homogeneous solution of the Langevin equation given in an explicit form in [10]. The limiting formula is valid in the infinite x limit as derived in [10]. Both at early and late times the factor $f \approx 1$, deviating from unity only for the time range of order $1/\omega_B$.

For discussion of a more general case of finite $V(\infty) < V_m$ we use the local, Ohmic approximation, which becomes excellent at late times. A potential that decreases fast at infinity as $x \to \infty$ is assumed; $\frac{dV}{dx} \to 0$. The acceleration term can then be neglected if $|\frac{d^2V}{dq_{\rm cl}^2}| \ll \eta^2$. This is a slow rolling approximation, and it always holds for x large enough. The classical equation is then solved as $\eta \int_{x_c}^{x} dz (\frac{dV}{dz})^{-1} = -\,t$, which gives the factor $f \approx -(\frac{dV}{dx_c})/(\eta p(\infty))$. Thus, the tunneling probability decreases with time along with the decreasing slope of the potential. Since the tunneling may not be terminated within a limited finite time, this result poses a curious question; there is a situation in the early universe in which the tunneling is never ended if the friction is strong.

We next turn to the case of $V(\infty) > V_m$, and consider the thermal initial state. At low temperatures of $T \ll V_h$ the dominant contribution comes from the energy range $0 < E < V_h$. Contribution from the subbarrier region in q_i integration is small and may be ignored. We add two contributions from the left well and from the overbarrier region. In the left well region the Wigner function is given by

$f_W^{(i)}(q_i\,,p_i) \propto \exp[-\tanh(\beta\omega_*/2)(\omega_* q_i^2 + p_i^2/\omega_*)]$. It is more appropriate here to compute the transition probability by $\sim \int dp\, f_W^{(R)}(x\,,p\,;t)$, without the flux p factor. The final position x is taken around x_0 of width Δx. If one makes a rough approximation for both the left well and the overbarrier region by harmonic oscillators, the relevant classical motion is given by a linear function of initial values, $q_i\,, p_i$, reducing the phase space integral to a restricted Gaussian type.

The averaged tunneling probability over Δx (Gaussian weight assumed) is $\frac{1}{\sqrt{\pi A}} \exp\left(-\frac{x_0^2}{A}\right)$ from the left well region, with $A = (\frac{g_1^2}{\omega_*} + \omega_* g_2^2)\coth(\frac{\beta\omega_*}{2}) + 2(\Delta x^2 + I_{11})$, where $g_i(t)$'s are two independent solutions to the linearized equation in the left well. The time averaged value over $\Delta t \gg 1/\omega_*$ gives $\overline{g_1^2} \approx \frac{1}{2}e^{-\eta t}$, and $\overline{g_2^2} \approx e^{-\eta t}/(2\omega_*^2)$, in the weak coupling. In the late time limit $I_{11} \approx \coth(\beta\omega_*/2)/(2\omega_*)$, and the exponent factor becomes of order, $\exp[-\omega_* x_0^2/(1 + 2\omega_*\Delta x^2)]$ at $T \ll \omega_*$, while at $T \gg \omega_*$ it is $\exp[-\omega_*^2 x_0^2/(2T + 2\omega_*^2\Delta x^2)]$.

On the other hand, one may use the WKB form of the wave function in the overbarrier region, with the transmission coefficient $|T(E)|^2 = e^{-\,2\pi(V_h - E)/\omega_B}$, using the inverted harmonic oscillator of the curvature ω_B for the subbarrier region. The density matrix $\rho_q^{(i)}(q\,,q')$ is then ($T \gg \omega_*$ is assumed)

$$\beta\omega_* e^{-2\pi V_h/\omega_B} \int_0^{V_h} dE\, \exp\left[-(\beta - \frac{2\pi}{\omega_B})\,E\right]\, \varphi(q\,;E)\varphi^*(q'\,;E)\,, \qquad (18)$$

where $\varphi(q\,;E) \approx \cos(\int_{x_*}^{q} dx\, p(x\,;E) - \frac{\pi}{4})/\sqrt{p(q\,;E)}$. The contribution from the overbarrier region is then roughly $\beta\omega_*(e^{-2\pi V_h/\omega_B} - e^{-\beta V_h})/(\,(\beta - 2\pi/\omega_B)(\omega_0\sqrt{2\pi\Delta x^2 + \pi\coth(\beta\omega_0/2)/\omega_0}\,)\,)$. In the case of overdamping this asymptotic value is approached from below by a slowly varying term $\propto e^{-2\omega_0^2 t/\eta}$. Since $\omega_* x_0^2 \gg V_h$ and $\omega_* = O[\omega_B]$, these contributions from the overbarrier region are generally larger than those from the left well region. One should compare this with the zero temperature result, $\omega_* e^{-2\pi V_h/\omega_B}/(\omega_0\sqrt{2\pi\Delta x^2 + \pi/\omega_0})$ in order to assess the effect of dissipative medium.

In summary we gave a real-time formulation of tunneling dynamics in thermal medium within the semiclassical framework.

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Figure caption

Fig.1

Two types of tunneling potential.